Three-body Interactions in One Dimension

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We determine the phase-diagram of a one-dimensional system of hard-core lattice bosons interacting via repulsive three-body interactions by analytic methods and extensive quantum Monte-Carlo simulations. Such three-body interactions can be derived from a microscopic theory for polar molecules trapped in an optical lattice. Depending on the strength of the interactions and the particle density, we find superfluid and solid phases, the latter appearing at an unconventional filling of the lattice and displaying a coexistence of charge-density-wave and bond orders.

INTRODUCTION

Quantum many-body systems provide a wealth of fascinating phenomena in condensed matter physics, including superfluidity in liquid Helium, the fractional quantum Hall effect, as well as the exotic electronic states in the pseudogap regime of cuprate superconductors. While these quantum phases emerge from dominant two-body interactions, with higher-order many-body interaction terms providing only small corrections, an exciting recent avenue of research in atomic and molecular physics is to engineer systems where higher-order interactions dominate. In particular, it was recently shown that this goal can be achieved for three-body interactions using polar molecules [1]. In the present work, we study the most fundamental model Hamiltonian which displays three-body interactions in one dimension via quantum Monte-Carlo simulations.

One-dimensional bosonic systems in the strongly correlated regime have recently been realized with cold atomic gases: examples are the superfluid/Mott-insulator quantum phase transition for atoms trapped in optical lattices [2], [3], and the cross-over into the hard-core (Tonks-Girardeau) regime [4]. A characteristic feature of hard-core bosons in a lattice with additional off-site two-body interactions is the appearance of solid phases at half-filling $n = 1/2$ with either a charge-density wave (CDW) or a bond-ordered (BOW) phase [5], [6].

In contrast, here we study hard-core bosons with strong three-body interactions. While the microscopic realization of the model with polar molecules gives rise to next-nearest-neighbor two-body and three-body interactions [1], the dominant part of the Hamiltonian is

$$H = -J \sum_i \left[b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger \right] + W \sum_i n_{i-1} n_i n_{i+1}. \quad (1)$$

The first term describes the standard kinetic energy with hopping rate J, while the second term, accounts for the three-body interaction with strength W; $n_i = b_i^\dagger b_i$ is the density operator with bosonic operators b_i and $b_i^\dagger$ satisfying the hard-core constraint. A similar model has recently been studied in two-dimensions [7].

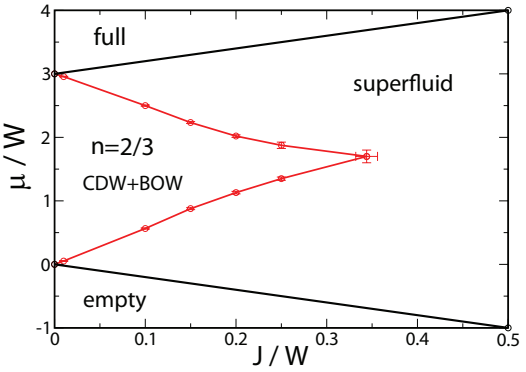

FIG. 1: (Color online) (QMC method: WA) Phase-diagram of hard-core lattice bosons with dominant three-body interactions, Eq. (1), in the grand-canonical ensemble, μ/W vs J/W. The solid phase at filling $n = 2/3$ is characterized by a coexistence of CDW and BOW orders.

We derive the complete quantum phase diagram of Hamiltonian (1) by means of extensive quantum Monte-Carlo simulations. We find the existence of both superfluid (SF) and solid phases, see Fig. 1. However, in contrast to systems with two-body interactions, we show that the solid phase appearing at the unconventional filling $n = 2/3$ exhibits both CDW and BOW orders. While Luttinger liquid theory predicts also instabilities towards a solid phase at $n = 1/2$ and $n = 1/3$, we show here that the system remains superfluid even for strong three-body interactions $W/J \gg 1$. Solid phases at filling $n = 1/2$ are found by adding *weak two-body* nearest-neighbor (NN) and next-nearest-neighbor (NNN) corrections to Eq. (1), $V_1 \sum_i n_i n_{i+1}$ and $V_2 \sum_i n_i n_{i+2}$ respectively, as naturally realized with polar molecules [1].

RESULTS

The ground state phase diagram of the model in Eq. (1) is derived in the grandcanonical ensemble by varying the

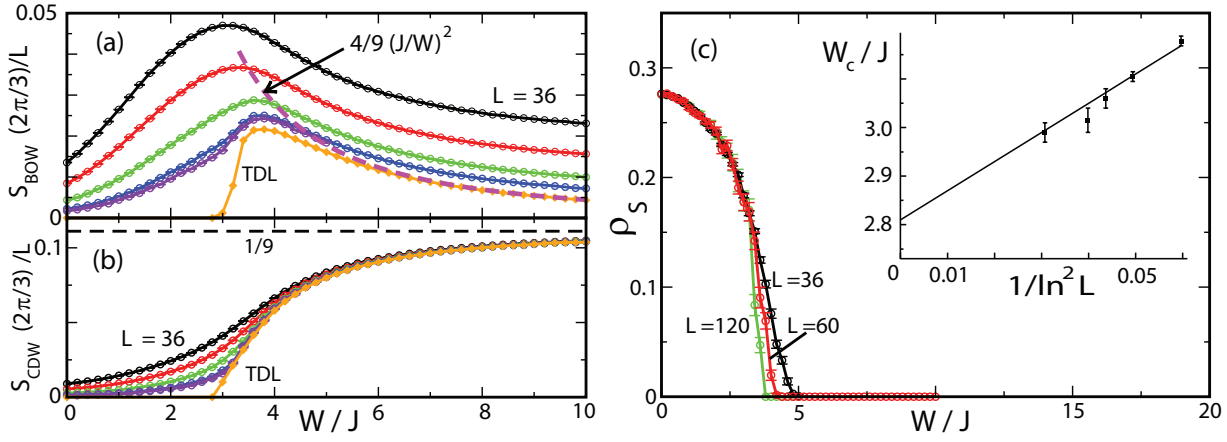

FIG. 2: (Color online) (QMC method: SSE) *Lattice filling* $n = 2/3$. (a) Bond-order structure factor $S_{\rm BOW}(2\pi/3)/L$ vs W/J. Top to bottom: lattice sizes $L = 36, 60, 120, 240$ and 300; the thermodynamic limit (TDL) is indicated. Dashed line: strong coupling perturbative result $4/9(J/W)^2$. (b) Density structure factor $S_{\rm CDW}(2\pi/3)/L$ vs W/J. Top to bottom: lattice sizes $L = 36, 60, 120, 240$ and 300; the TDL is indicated. Dashed line: strong coupling result $n^2/4 = 1/9$. (c) Superfluid density ρ_s as a function of W/J, for lattice sizes $L = 36, 60$ and 120. Inset: $W_{\rm c}/J$ as a function of $1/\ln^2 L$, results from the WA. The line is a guide to the eye.

chemical potential μ at different fixed values of W/J. We use two different quantum Monte-Carlo (QMC) methods: (i) the stochastic series expansion (SSE) algorithm with a generalized directed loop update [8] after a decoupling of the Hamiltonian in trimers for each tree-body interaction term, and (ii) a code based on the Worm algorithm (WA) path integral approach [9], which allows efficient sampling of the many-body path winding numbers in imaginary time and space directions. Although the SSE method samples both BOW and CDW orders, its efficiency drops for very large values of W/J. The WA does not suffer from this issue and is especially useful in checking the limit $W/J \gg 1$. Results obtained with the two methods are found to be consistent (see below). The groundstate properties of the finite systems have been probed using temperatures $T = 0.6J/L$, with L the number of lattice sites, which was found sufficiently low.

The phase diagram is determined by two phases, see Fig. 1: a superfluid Luttinger liquid (LL) phase with algebraic correlations, surrounding a solid phase at filling $n = 2/3$, which appears for dominant three-body interactions $W/J \gtrsim 3$. The solid phase is incompressible, giving rise to the characteristic lobe structure in the μ-W phase diagram. This incompressible phase is characterized by the structure factors $S_{\rm CDW}$ for a charge density wave and $S_{\rm BDW}$ for a bond order at the wave-vector $k = 2\pi/3$

$$S_{\rm CDW}(k) = \frac{1}{L}\sum_{j,l} \exp\left[ik\,(j-l)\right]\langle n_j n_l\rangle, \qquad (2)$$

$$S_{\rm BOW}(k) = \frac{1}{L}\sum_{j,l} \exp\left[ik\,(j-l)\right]\langle K_j K_l\rangle, \qquad (3)$$

with the bond operators $K_l = b_l^\dagger b_{l+1} + b_l b_{l+1}^\dagger$.

The presence of CDW order can be easily understood in the limit $J = 0$, where the ground state at filling $n = 2/3$ is threefold degenerate. In fact, up to lattice translations, each groundstate takes the form $|\Omega\rangle = \prod_k b_{3k}^\dagger b_{3k+2}^\dagger |0\rangle$, and exhibits CDW order with $S_{\rm CDW}(2\pi/3) = n^2 L/4$. From the unconventional filling $n = 2/3$ of the solid phase, it follows that once hopping of particles is allowed the charge density order implies small hopping correlations, since the position of a particle in the solid breaks the symmetry of hopping to the left or hopping to the right. Using standard perturbation theory in the hopping term, we find that also a bond order wave appears for finite hopping with $S_{\rm BOW}(2\pi/3) = n^2 L J^2/W^2$. Monte Carlo results directly confirm the coexistence of the two orders. Analogous to the case of the Hubbard-model with onsite two-body interactions, this incompressible phase at filling $n = 2/3$ can be reached by varying the density, which corresponds to a mean-field transition, or by keeping the density constant and by varying the strength of the interactions W/J, see Fig. 1. We found that the superfluid density vanishes at the boundaries, indicating that doping of the system happens simultaneously to the solid/SF transition. In the following we will be mainly interested in characterizing the constant-density transition at the tip of the lobe.

Filling $n = 2/3$

Our results for the order parameters $S_{\rm BOW}$ and $S_{\rm CDW}$ at fixed density $n = 2/3$ are shown in Fig. 2 for system sizes

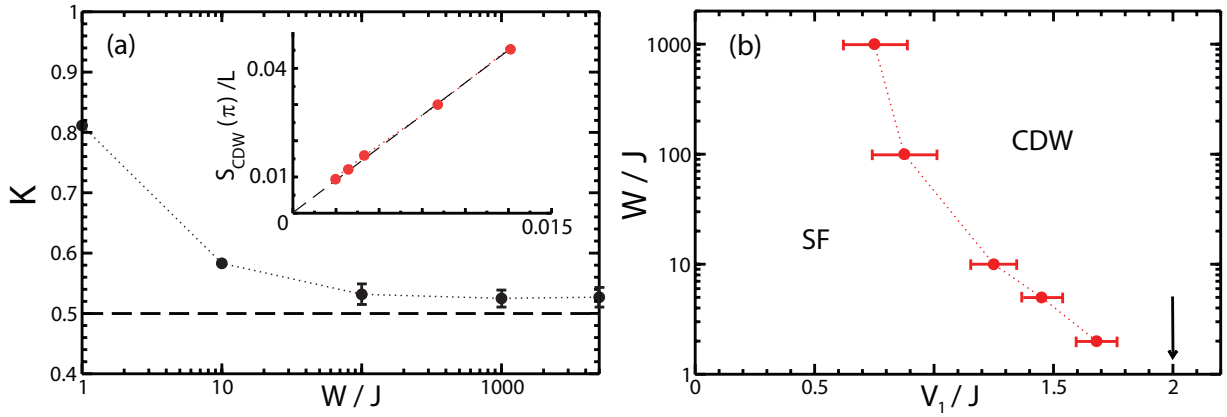

FIG. 3: (Color online) (QMC method: WA) *Lattice filling* $n = 1/2$. (a) Luttinger Liquid parameter K as a function of W/J with critical value $K_c = 0.5$ (dashed line) of the superfluid/solid transition. The inset shows the density structure factor $S_{\rm CDW}(\pi)/L$ as a function of the inverse system size $1/L$ for $W/J = 1000$. (b) Phase diagram in the presence of an additional nearest neighbor interaction V_1 in the plane W/J vs V_1/J. The arrow indicates the point of the superfluid/solid transition at $W/J = 0$.

$L = 36, 60, 120, 240$ and 300 (top to bottom), together with the extrapolated thermodynamic limit (TDL) behavior. The latter has been obtained based on an observed linear scaling of $S_{\rm BOW}$ and $S_{\rm CDW}$ in $1/L$ within the solid phase, and is found to be in perfect agreement with the strong-coupling results for the order parameters valid for $W/J \gg 1$ (dashed lines). In the thermodynamic limit, the two order parameters are found to vanish simultaneously at a critical ratio $W_c/J \approx 2.9$, corresponding to the solid/liquid transition at the tip of the lobe.

A more refined determination of the transition point can be obtained using bosonization techniques. In the weakly interacting regime with $W/J \ll 1$, the system can be mapped onto the sine-Gordon model [1]

$$H = \frac{\hbar v}{2} \int dx \left\{ \left[K\Pi^2 + \frac{1}{K} \left(\partial_x \Phi\right)^2 \right] + \lambda \cos(\gamma \Phi) \right\}, \quad (4)$$

where Φ denotes the charging field and Π the canonical conjugate operator, while K is the LL parameter, and $\gamma = \sqrt{36\pi}$ the periodicity of the sine-term. Consequently, the transition from the LL to the solid phase at the tip of the lobe in Fig. 1 appears at the critical value $K_c = 2/9$ and it belongs to the Kosterlitz-Thouless (KT) universality class. For weak interactions $W/J \ll 1$ the behavior of the Luttinger parameter is obtained directly from bosonization techniques as $K = 1 - (2\sqrt{3}/\pi)W/J$, however this value is strongly renormalized close to the liquid/solid quantum phase transition. We compute the LL parameter numerically as $K = \hbar\pi\sqrt{\rho_s \kappa/m}$ by QMC methods, with ρ_s and κ the superfluid density and compressibility, respectively. The latter are calculated from the statistics of winding numbers $\langle W_\alpha^2 \rangle$ in imaginary time and space directions. In particular, for a square system such that $L_\tau \approx L_x = L$, with $L_\tau = \hbar v/T$ and $v = \sqrt{\rho_s/\kappa m}$ the sound velocity, $\rho_s = mLT\langle W_x^2\rangle/\hbar^2$ [10], and $\kappa = \langle W_\tau^2\rangle/LT$, respectively, with $m = \hbar^2/2J$. We have performed simulations for $L = 60, 90, 120, 150$ and 300. In order to precisely locate the critical point we employ finite size scaling arguments following from the KT renormalization group flow [11]. Calling $W_c(L)$ the value of W for which $K(L) = K_c$, the finite size scaling of the transition point is $W_c(L) - W_c \propto [\ln(L)]^{-2}$, with W_c the transition point in the thermodynamic limit. The inset in Fig. 2(c) shows the finite size scaling of $W_c(L)$, which gives the transition point $W_c/J = (2.80 \pm 0.15)$, in agreement with the discussion above.

Filling $n = 1/2$

In Ref. 1 it is argued that for lattice filling $n = 1/2$ a superfluid/solid transition should occur as a function of W/J at a critical LL parameter $K_c = 0.5$. This instability is based on the observation that replacing the density operator by its fluctuations around the mean value $n_i = n + \delta n_i$, the three-body interaction gives rise to a nearest neighbor and next-nearest neighbor interaction,

$$W \sum_i n_{i-1} n_i n_{i+1} \sim Wn \sum_i \left[\delta n_{i-1} \delta n_{i+1} + 2\delta n_{i-1} \delta n_i \right].$$

In analogy to systems with two-body interactions, one would expect a solid phase at half-filling $n = 1/2$. However, we find that the competition between the nearest-neighbor interaction of strength $2Wn$, which drives an instability towards a CDW solid, and the next-nearest neighbor interaction of strength Wn, which drives an instability towards a BOW solid, removes all instabilities altogether, see below. The low-temperature phase is thus a superfluid, independent of the magnitude of W/J.

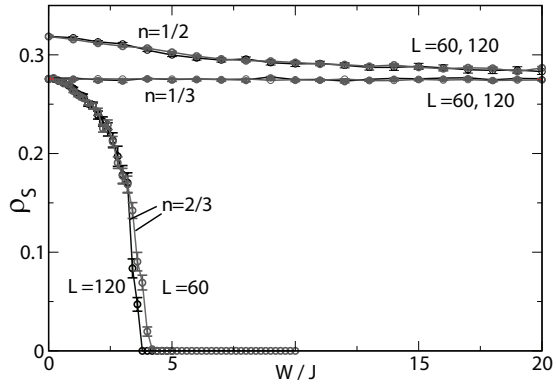

FIG. 4: (QMC method: SSE) Superfluid fraction ρ_s as a function of W/J for fillings $n = 1/3, 1/2$ and $2/3$. Grey and black lines correspond to system sizes $L = 60$ and 120, respectively. Due to particle-hole symmetry, the superfluid fractions for $n = 1/3$ and $2/3$ are the same for $W/J = 0$.

This behavior is a special property of three-body interactions, and it is in stark contrast to the two-body case, where a transition into the solid phase has been always reported [5]. In Fig. 3(a) we show our results for K as a function of W/J, obtained using the procedure described above for system sizes $L = 80, 120, 160, 240$ and 320. For weak three-body interactions $W/J \lesssim 1$, K tends to the hard-core value $K = 1$. We find that for large interactions $W/J \gg 1$ the LL parameter saturates at a value $K = (0.528 \pm 0.015) > K_c$ which is larger than the critical value $K_c = 0.5$, and thus no superfluid/solid transition occurs at filling $n = 1/2$. Consistently, the superfluid fraction does not show any appreciable system-size dependence, Fig. 4.

The inset of Fig. 3(a) shows the structure factor $S_{\rm CDW}(\pi)$ as a function of the inverse system size $1/L$, for the case of $W/J = 1000$. The structure factor extrapolates to a value consistent with zero in the termodynamic limit, consistent with a superfluid in this limit of large three-body interactions. It remains an open question, whether there is an analytical result predicting the value of the Luttinger parameter for infinite three-body interactions in analogy to hard-core bosons with $K = 1$.

Additional two-body interactions

We finally consider the effects of additional short-ranged two-body repulsions, by adding to the model in Eq. (1) a term $V_1 \sum_i n_i n_{i+1} + V_2 \sum_i n_i n_{i+2}$ with nearest neighbor (NN) repulsion V_1, and next-nearest-neighbor (NNN) repulsion V_2. Such terms are important as they constitute the leading correction to the short-range three-body repulsions considered thus far, and can induce new instabilities of the LL. In fact, it is well known that a half-filled system of hard-core bosons with NN repulsions V_1 undergoes a superfluid/CDW KT transition at $V_1 = 2J$ to a two-fold degenerate state with ordering pattern $\circ\bullet\circ\bullet$ ($k = \pi$) [12].

In Fig. 3(b) we show how this transition is modified due to the presence of three-body interactions, by presenting the low-energy phases as a function of W/J and V_1/J. We find that the presence of three-body interactions renormalizes considerably the SF/CDW transition by shifting it to lower values of $V_1/J < 2$. In particular, for $W/J = 1000$ we find $V_1^c/J = (0.75 \pm 0.15)$.

The presence of NNN interactions $V_2 > 0$ can drive the system into a bond-ordered phase. In Ref. 5 it is shown that an ensemble of hard-core bosons with NNN-interactions (at $V_1 = 0$) enters a $k = \pi$ bond-ordered phase for $V_2/J = (2.15 \pm 0.10)$. For even larger $V_2/J > (2.66 \pm 0.10)$, a four-fold degenerate $k = \pi/2$ CDW phase with ordering pattern $\circ\bullet\bullet\circ$ becomes stabilized. We find that the presence of three-body interactions significantly renormalizes these transition points. For example, at $W/J = 10$ the SF/BOW transition occurs for $V_2/J = (0.9 \pm 0.1)$, and the BOW/CDW transition at $V_2/J = (2.1 \pm 0.1)$. Three-body interactions thus widen the extent of the BOW phase in this regime.

Filling $n = 1/3$

We find that at filling $n = 1/3$ the low-energy phase remains a superfluid independently of the strength of the three-body interactions. Consistently, the superfluid fraction ρ_s in this case is found to be essentially independent of W/J in the range $0 < W/J < 20$, as seen in Fig. 4. We computed the value of the LL parameter for $W/J = 1000$, and found that $K = (0.89 \pm 0.01) > K_{\rm c} = 2/9$, which confirms that three-body interactions alone do not induce a transition in this region. This finding contrasts the weak-coupling result Ref. 1, and exhibits the strong breaking of particle-hole symmetry by finite three-body interactions, as seen for $W \neq 0$ from e.g. comparing ρ_s for the two fillings $n = 1/3$ and $n = 2/3$ in Fig. 4. Adding a NN interaction also does not induce any transition at $n = 1/3$. In fact, we find for $W/J = 1000$ and $V_1/J = 20$ that $K = (0.48 \pm 0.01) > K_{\rm c}$.

CONCLUSIONS

We have determined the phase diagram of the fundamental model Hamiltonian for hard-core bosons with dominant short-range three-body interactions in one dimension. The latter can be realized with polar molecules cooled to the electronic and vibrational groundstate, which is well in the reach of current experiments [13]. The one-dimensional nature of the problem opens fascinating prospects for studying the dynamics of systems with many-particle interactions by using powerful numerical

techniques such as e.g. tDMRG [14]. Extensions to two dimensions [7] in various lattice geometries hold promises in the search for exotic phases, such as e.g. topological phases and spin liquids.

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